

1-Dodecyl-2-methylpyridin-1-ium iodide
14402-22-3 | DTXSID60506018

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 7.23e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.71e-01

Confidence level: 8.60e-01

Nearest Neighbors from the Training Set

Image not found

alpha-Phellandrene

Measured: 3.13e-10

Predicted: 2.83e-10

Image not found

(2E)-2-Hexenal

Measured: 4.40e-11

Predicted: 4.31e-11

Image not found

(3Z)-3-Hexenyl acetate

Measured: 7.80e-11

Predicted: 7.52e-11

Image not found

Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

Measured: 4.80e-11

Predicted: 4.73e-11